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Critical behaviour in QCD at finite isovector chemical potential

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We report an investigation of criticality in QCD at finite isovector chemical potential, μ_3, and at zero temperature. At the critical point, $\mu_3^c \approx m_\pi$, we find that an uncharged scalar and pseudoscalar and a charged pseudoscalar meson become massless within the resolution of our measurement. The effective long distance theory therefore breaks $O(4)$ symmetry by charged pion condensation. This results in a rising quark number susceptibility. The baryon remains massive, as indicated by a vanishing baryon number susceptibility.

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In the last few years there has been a resurgence of interest in the phase diagram of QCD [1]. Perturbation theory and effective chiral models have been used to uncover a rich phase structure at finite chemical potential and low temperatures [2]. This region of non-vanishing baryon chemical potential remains out of reach of present lattice computations, due to the Fermion sign problem [3]. However, the same techniques, namely effective chiral models and perturbation theory, have also been used to investigate the phase structure for non-vanishing isovector chemical potential [4]. This new direction in coupling space is amenable to lattice computations, which can therefore test the various methods applied to computations at finite baryon chemical potential.

It is clear that the Dirac operator, M, is non-negative if $M^\dagger = QMQ^{-1}$ for some operator Q. For two-flavour QCD with isovector chemical potential,

$$M = \begin{pmatrix} D(\mu_3) & 0 \\ 0 & D(-\mu_3) \end{pmatrix} \qquad \text{and} \qquad Q = \gamma_5 \otimes \tau_2, \tag{1}$$

the action is positive definite provided each flavour satisfies γ_5-hermiticity ($D^\dagger = \gamma_5 D \gamma_5$) and the quark masses are degenerate [5]. The phase diagram of this model was investigated by chiral perturbation theory and by perturbative QCD and a second order phase transition in the $O(4)$ universality class was found at $\mu_3 = m_\pi$ due to the condensation of charged pions [4]. A first quenched lattice investigation of this model has been reported recently [6] and a phase transition due to pion condensation has indeed been found. When $\det M$ is real and positive, quenching does not produce the pathologies which can otherwise arise.

We show here that it is possible to determine the symmetry of the problem, and through universality then predict the critical exponents, by investigating the spin-flavour content of the massless particles in the theory. Our quenched computations verify that a second order phase transition occurs at $\mu_3 = m_\pi$. At, and above, the critical point the scalar σ, the neutral pion and one linear combination of charged pions becomes effectively massless. This lends support to the idea that the effective field theory should have an $O(4)$ symmetry broken down by giving mass to a charged pion, *i.e.*, by pion condensation. If one is so inclined, this can be further tested by the usual, more expensive, method of finite-size scaling. However, as pointed out in [6], this is non-trivial since higher dimensional operators in the lattice theory are important at the cutoffs which are presently accessible. These could easily influence the effective exponents seen. Scaling studies become then many-fold more difficult due to the necessity of taking finer lattices before investigating finite volume effects.

The partition function of two-flavour QCD is

$$Z = \int \mathcal{D}U e^{-S_W} \det M(m_u, \mu_u) \det M(m_d, \mu_d), \tag{2}$$

where S_W is the Wilson gauge action and each determinant corresponds to one flavour of quarks. At the moment we are interested in the case when $m_u = m_d = m$. The chemical potentials for each flavour can be combined into the baryon and isovector chemical potentials $\mu_0 = 3(\mu_u + \mu_d)/2$ and $\mu_3 = (\mu_u - \mu_d)/2$ respectively. It is instructive to invert these relations and write

$$\mu_u = \frac{\mu_0}{3} + \mu_3, \qquad \mu_d = \frac{\mu_0}{3} - \mu_3. \tag{3}$$

We shall work with $\mu_0 = 0$ and $\mu_3 > 0$. Since the identification of u and d quarks is arbitrary in the absence of electroweak interactions, the difference between positive and negative μ_3 is purely conventional. A flip in the sign of μ_3, as preferred in [4], can be accomplished by just interchanging our definitions of u and d quark flavours.

Quantum number densities are defined as

$$n_i \equiv \left(\frac{T}{V_3}\right) \frac{\partial \ln Z}{\partial \mu_i}, \tag{4}$$

for $i = 0$ and 3. These are linear combinations of the quark number densities. The quantity n_3 is an order parameter for pion condensation. Other order parameters are the quark condensates $\langle\overline{\psi}\psi\rangle$ and $\langle\overline{\psi}\gamma_5\tau_2\psi\rangle$. At the expected phase transition $\langle\overline{\psi}\psi\rangle$ would depart from its vacuum value and $\langle\overline{\psi}\gamma_5\tau_2\psi\rangle$ would become non-zero. The added advantage in using n_3 is that it also flags the value of μ_3 at which saturation sets in, with every site of the lattice being filled to capacity with quarks, and continuum physics can no longer be extracted.

The quark number susceptibilities [7], $\chi_{ij} = \partial n_i/\partial\mu_j$ can also be used to probe the transition. The flavour off-diagonal susceptibility is given by

$$\chi_{ud} = \left(\frac{T}{V_3}\right)\Big[\left\langle \mathrm{tr} M_u' M_u^{-1}\, \mathrm{tr} M_d' M_d^{-1}\right\rangle - \left\langle \mathrm{tr} M_u' M_u^{-1}\right\rangle \left\langle \mathrm{tr} M_d' M_d^{-1}\right\rangle\Big]. \qquad (5)$$

This differs from the usual $\mu_f = 0$ expression [8] through the subtraction of the last term, corresponding to non-vanishing quark densities. When a charged pion condensate forms, χ_{ud} must become non-zero and negative. Expressions for the flavour diagonal susceptibilities can be read off from [8] and modified by appropriate subtraction of the non-vanishing quark number densities. As long as the baryon remains massive, $\chi_0 = \partial n_0/\partial\mu_0$ should remain zero. χ_3 is a combination of χ_0 and χ_{ud} and hence gives no extra information.

We explicitly use two staggered quark fields— one for each component of the Fermion matrix in eq. (1). We adopt and extend the usual "cure" for Fermion doubling, and write the two-flavour (one up and one down) determinant as

$$\det M = (\det M_u M_d)^{1/4}. \qquad (6)$$

Consequently, each trace in eqs. (4,5) comes with a factor of 1/4 multiplying it. There are two ways in which quark masses enter the problem— the sea quark mass appears in the determinants in eq. (2) and influence the path integral measure, while the valence quark mass enters into the operators such as in eq. (5). In the quenched approximation the determinants are set to unity, so the sea quarks drop out of the problem but not the valence quarks.

It might seem that the use of staggered quarks is a needless complication since the number of mesons of any given spin is much larger than that expected in two flavour QCD. However, only four of these are Goldstone pions at $T = \mu = 0$. The others are split from them at any finite lattice spacing. This trick gives us the ability to bypass some of the problems seen at coarse lattice spacing. On finer lattices the number of Goldstone modes for staggered quarks is in any case a problem in defining two staggered flavours and some other formulation of lattice quarks is probably better suited to the problem. One other advantage to using two independent staggered quark fields is that it allows us to give them unequal masses if we so wish.

The partition function of eq. (2) can be expressed through a transfer matrix— $Z = \mathrm{Tr} T^N(T, \mu_0, \mu_3)$. The transfer matrix T propagates field information from one slice of the lattice to another, and N is the number of slices. There may be several inequivalent ways to slice the lattice, giving rise to possibly inequivalent transfer matrices, but the partition function is unique. The eigenvalues of T, $\lambda_0 \geq \lambda_1 \geq \cdots$, define masses (or screening masses) through the formula $1/m_i = \log(\lambda_0/\lambda_i)$. A critical point implies massless modes for all the transfer matrices. We utilise the transfer matrix in the time direction and determine the spin-flavour content of massless mesons which propagate in the time direction.

Since the theory at finite chemical potential has a conjugate quark [9], the symmetries of the transfer matrices must take this into account. In the problem at hand, there are two staggered quark fields which are conjugate to each other. The symmetry group at $T = \mu = 0$ therefore contains an extra $SU(2)$ factor corresponding to arbitrary rotations between these two fields. This symmetry is broken at finite μ. Recall that a chemical potential enters the lattice Dirac operator, M, through the time component of the covariant derivative because every temporal gauge field is multiplied by the fugacity, $\exp(a\mu)$. As a result, for finite μ_3, the $Z(2)$ group generated by $t \to -t$ does not commute with the new $SU(2)$. The symmetry of the transfer matrix can be constructed by flipping the roles of the two quarks when flipping the sign of time. The irreps can be constructed by taking Z_2 invariant combinations such as $\pi^0_\pm = \bar{u}\gamma_5 u \pm \bar{d}\gamma_5 d$ and $\pi^- = \bar{u}\gamma_5 d$ or $\pi^+ = \bar{d}\gamma_5 u$. When electroweak corrections are neglected, as is the case here, one can also use the linear combinations $\pi_\pm = \bar{u}\gamma_5 d \pm \bar{d}\gamma_5 u$. The irrep labels of [10] can be retained with a reinterpretation of the old time-reversal quantum number as the product of time-reversal and the Z_2 flip of the up and down quarks above [11].

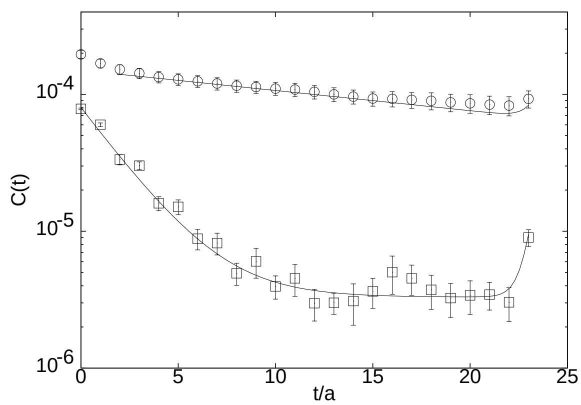

FIG. 1: The correlators for the $\overline{d}d$ part of π^0 (circles) and σ (boxes) for $a\mu_3 = 1$ on a 24×8^3 lattice. The lines are fits to the spin projected part of the $\overline{u}u$ projection and rotated in flavour according to the symmetry of the transfer matrix.

The importance of identifying the irreps of the transfer matrix follows from an observation made in [13]: on any finite lattice an unphysical mode of propagation for a meson is that a quark and an antiquark travel in opposite directions around the lattice. This finite size effect is rendered innocuous at $\mu = 0$ by proper importance sampling. However, a chemical potential exacerbates this problem by encouraging forward propagation of the quark and backward propagation of the same flavour of the anti-quark. The correlation function of a pure flavour state is no longer symmetric in t, but has the form

$$C(t) = A\mathrm{e}^{-mt} + A'\mathrm{e}^{-m'(N_t-t)}, \qquad (7)$$

with $m \neq m'$, which seems to indicate the absence of a transfer matrix. However, by recombining flavours into the irreps of the symmetries of the transfer matrix we recover the correct symmetric form.

In Figure 1 we show an example of this. Note that masses fitted to such pure flavour correlators by the formula in eq. (7) are still useful, since the transfer matrix eigenstates (which are linear combinations of flavours) have the same masses. Tests of mass fits therefore include the check that the roles of the parameter pairs (A, m) and (A', m') are flipped when fitting the $\bar{u}u$ and $\bar{d}d$ correlators, and that the eigenstates of the transfer matrix do, in fact, give the lower of these two masses. Figure 1 does, in fact, show one such test, since the correlation functions plotted are the $\overline{d}d$ type, and the fits shown are plotted using parameters obtained from the $\overline{u}u$ type and flipped. We have further checked that local masses also show a plateau close to this mass.

We have simulated quenched QCD on 8^4 and 12^4 lattices at $\beta = 5.8941$, which is the critical coupling for the finite temperature transition in quenched QCD with 6 time slices. The lattice spacing is then fixed to be $a = 1/6T_c$. In the quenched theory, since $T_c/\Lambda_{\overline{MS}} = 1.15\pm0.05$ [14], the lattice cutoff is $a^{-1} = (6.9\pm0.3)\Lambda_{\overline{MS}}$. The two lattice sizes differ by 50% in linear extent. This is necessary to see and control gross finite volume distortions, but not sufficient to perform a study with the finesse required to extract critical indices from finite size effects. We have generated 40 stored configurations for analysis on the smaller lattice and 70 on the larger. These are obtained with a Cabbibo-Marinari pseudo-heatbath algorithm where each $SU(2)$ subgroup imbedded in $SU(3)$ is touched thrice during every link update. An initial 5000 sweeps are discarded for thermalisation and each subsequent stored configuration is separated from the previous one by 1000 sweeps. The successive stored configurations are therefore fully decorrelated from each other, rendering the analysis of measurement errors fairly simple.

Our methods for measuring the number densities and susceptibilities are the same as in [8]. The chiral condensate is measured from the same matrix inversions. Correlators are obtained with a point source and projected on to zero 3-momentum by summing over the sink. The spectrum measurements use standard techniques for staggered quarks, including fitting to and extracting local masses from spin-projected parts of the correlators. Since we work on finite lattices, we have a finite resolution for the identification of massless modes. When a mass reaches the value $1/aN_t$, the corresponding particle becomes effectively massless and contributes to the long-distance effective theory.

Since this is a first survey, we chose to work with a reasonably heavy valence quark mass— $ma = 1/6$. At $T = \mu_3 = 0$ this gave $m_\pi a = 1.065 \pm 0.003$ and $m_\rho a = 1.323 \pm 0.007$. The baryon mass was $m_p a = 1.59 \pm 0.05$. These measurements are compatible with previous computations at nearby couplings [15]. Since $m_\pi L \approx 12$ on our larger lattice, we expect finite volume distortions to be small at this quark mass except in the neighbourhood of any critical point, where, in any case, we expect to see other physics as already explained.

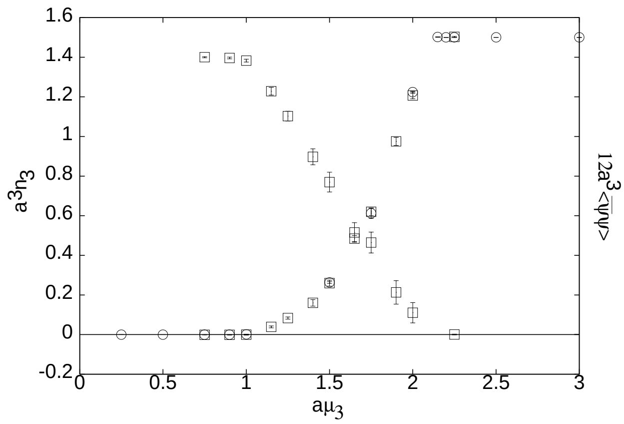

FIG. 2: The order parameters. Boxes denote measurements on 8^4 lattices and circles those on 12^4 lattices.

Measurements of the order parameters as functions of μ_3 are shown in Figure 2. We draw attention to two salient facts. First, $\langle\overline{\psi}\psi\rangle$ and n_3 both depart from their vacuum value at the same $a\mu_3^c \approx 1 \approx am_\pi$, and, second, the two lattice sizes yield identical results for the critical μ_3^c. From the flattening of n_3 at $a\mu_3 \approx 2$ it is clear that saturation sets in and continuum physics can no longer be extracted. The critical point is reached far before this. The susceptibility χ_{ud} is zero at $T = \mu_3 = 0$ [8]. It begins to depart from this value, becoming negative, soon after μ_3^c. Its behaviour is closely related to the massless combination of charged pions. Throughout this range of μ_3, n_0 is consistent with zero, indicating that the baryon remains massive [16].

Figure 3 shows the μ_3-dependence of masses of the π_+^0 and σ_+ obtained from zero-momentum correlators. The masses of the σ_+ and π_+^0 drop rapidly from their $T = 0$ values and become nearly massless close to $a\mu_3^c$. They remain massless till saturation sets in. The π_+ mass is

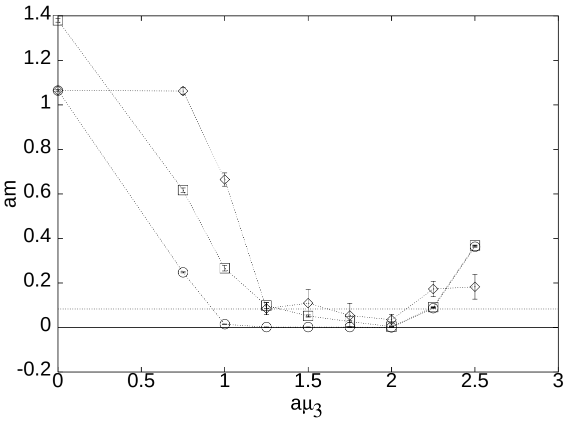

FIG. 3: The spectrum of π^0_+ (circles), σ_+ (boxes) and π_+ (diamonds) obtained from temporal correlators on 12^4 lattices. The horizontal dotted line indicates the mass resolution available on a lattice of this size.

the most interesting. It is non-zero at $\mu_3 = 0$ due to the finite quark mass and degenerate with the π^0_+. It does not change appreciably till μ_3^c, at which point it drops rapidly and becomes effectively massless soon after. The higher of the two masses in the flavour projected charged pion sector, corresponds to π_-. This remains non-zero in the whole range of μ studied here. All the critical behaviour seen in the order parameters is driven by this. The rise in meson masses in the unphysical region $a\mu_3 > 2$ is easy to understand: propagation of mesons is hard on a saturated lattice. This is also observed in a free field theory computation at large μ_3.

A few caveats need to be stated. At the resolution available at these lattice sizes, $a\mu_3^c$ can be observed to lie between 1 and 1.25, as seen in Figure 2. Figure 3 shows that the mass resolution available on the 12^4 lattice makes it unnecessary to improve the bounds on μ_3^c on this lattice. If one wants to nail down the critical isovector chemical potential with higher precision, then one must go to larger lattices, as always. We are presently exploring the pion-condensed phase in more detail with smaller quark masses and larger lattice volumes. These results, and the consequently more precise determination of μ_3^c will be presented elsewhere.

There are three notional regions of μ_3. Here we have explored the vicinity of $\mu_3 \approx m_\pi$ where we found that a chiral effective theory can be written. The region $\mu_3 \gg m_p$ is supposed to be the domain of validity of perturbation theory. This can be reached at either smaller lattice spacing or quark mass. The region $\mu_3 \approx m_\rho$ is not accessible to either effective theories or perturbative expansions, and a lattice computation is the only possible tool to explore this region. The extraction of the phase diagram in these qualitatively different regions of μ_3 is a major task, which we leave to the future.

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